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## Science & Emerging Technology of 2D Atomic Layered Materials and Devices

Angel Rubio

UNIVERSIDAD DEL PAIS VASCO - EUSKAL HERRIKO UNIBERTSITTEA

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Final Report

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<p><b>14. ABSTRACT</b>            The project resulted in 16 published papers in world-class journals and was instrumental, directly or indirectly, in the award of nine prestigious Marie Skłodowska-Curie grants to pursue follow-on research.            The papers that describe all the work are accessible in the attached document and are listed here:            - Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials. - h-AlN-Mg(OH)2 vdW Bilayer Heterostructure: Tuning the excitonic characteristics            - Emergent elemental two-dimensional materials beyond graphene. - Ab Initio Modeling of Plasmons in Metal-Semiconductor Bilayer Transition Metal Dichalcogenide Heterostructure            - Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry. - Confined linear carbon chains as a route to bulk carbyne            - On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: Intrinsic effects revealed from theory and experiment. - Square selenene and tellurene: novel group VI elemental 2D semi-Dirac materials and topological insulators. - Quantum Plasmonics: From jellium models to ab-initio calculations. - Negative plasmon dispersion in 2H-NbS2 beyond charge-density-wave interpretation            - Stable monolayer honeycomb-like structures of RuX2 (X = S, Se). - Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. - Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C60 and Polymer/SWNT Photovoltaic Devices. - Dynamics of observables and exactly solvable quantum problems: Using time-dependent density functional theory to control quantum systems.         </p>					
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March 8, 2017

Dear Dr. Mah,

Please find the attached forms SF-425-FFR and dd082, which constitutes the final reporting documents for AOARD project 144088, "2D Materials and Devices Beyond Graphene Science & Emerging Technology of 2D Atomic Layered Materials and Devices". These documents cover the grant period from February 19, 2016–February 18, 2017

We are proud to note that this AOARD funding contributed to the production of the following publications:

Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials

Hannes Hübener, Michael A. Sentef, Umberto De Giovannini, Alexander F. Kemper, Angel Rubio  
Nature Communications **7**, 13940 (2017)

h-AlN-Mg(OH)2 vdW Bilayer Heterostructure: Tuning the excitonic characteristics

C. Bacaksiz, A. Dominguez, A. Rubio, R. T. Senger, H. Sahin  
Physical Review B **(accepted)**, (2017)

Emergent elemental two-dimensional materials beyond graphene

Yuanbo Zhang, Angel Rubio, Guy Le Lay  
Journal of Physics D-Applied Physics **50**, 053004 (11pp) (2017)

Ab Initio Modeling of Plasmons in Metal-Semiconductor Bilayer Transition Metal Dichalcogenide Heterostructure

Huseyin Sener Sen, Lede Xian, Felipe Homrich da Jornada, Steven Louie, Angel Rubio  
Israel Journal of Chemistry, (2017)

Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry

Johannes Flick, Michael Ruggenthaler, Heiko Appel, Angel Rubio  
(2017)

Confined linear carbon chains as a route to bulk carbyne

L. Shi, P. Rohringer, K. Suenaga, Y. Niimi, J. Kotakoski, J.C. Meyer, H. Peterlik, M. Wanko, S. Cahangirov, A. Rubio, Z.J. Lapin, L. Novotny, P. Ayala, T. Pichler  
Nature Materials **15**, 634 - 639 (2016)

On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: Intrinsic effects revealed from theory and experiment

Dr. Bruce F. Milne, Christina Kjær, Jørgen Houmøller, Dr. Mark H. Stockett, Dr. Yoni Toker, Prof. Angel Rubio, Prof. Steen Brøndsted Nielsen  
Angewandte Chemie International Edition **128**, 6356 - 6359 (2016)

Square selenene and tellurene: novel group VI elemental 2D semi-Dirac materials and topological insulators

Lede Xian, Alejandro Pérez Paz, Elisabeth Bianco, Pulickel M. Ajayan, Angel Rubio  
Physical Review Letters **(Submitted)**, (2016)

Quantum Plasmonics: From jellium models to ab-initio calculations

Alejandro Varas, Pablo García-González, Johannes Feist, F. J. García-Vidal, Angel Rubio  
Nanophotonics **5**, 409 - 426 (2016)

## Negative plasmon dispersion in 2H-Nb<sub>2</sub>S beyond charge-density-wave interpretation

Pierluigi Cudazzo, Eric Müller, Carsten Habenicht, Matteo Gatti, Helmuth Berger, Martin Knupfer, Angel Rubio, Simo Huotari  
New Journal Of Physics **18**, 103050 (2016)

## Stable monolayer honeycomb-like structures of RuX<sub>2</sub> (X = S, Se)

Ersan, Fatih; Cahangirov, Seymur; Gokoglu, Gokhan; et al. Physical Review B 94, 155415 (2016)

## Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes

Duncan J. Mowbray, Alejandro Pérez Paz, Georgina Ruiz-Soria, Markus Sauer, Paolo Lacovig, Matteo Dalmiglio, Silvano Lizzit, Kazuhiro Yanagi, Andrea Goldoni, Thomas Pichler, Paola Ayala, Angel Rubio  
Journal Of Physical Chemistry C 120 (32), pp 18316–18322 (2016)

## Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C<sub>60</sub> and Polymer/SWNT Photovoltaic Devices

Livia Noemi Glanzmann, Duncan John Mowbray  
Journal Of Physical Chemistry C 120, 6336 - 6343 (2016)

## Dynamics of observables and exactly solvable quantum problems: Using time-dependent density functional theory to control quantum systems

Mehdi Farzanehpour, I. V. Tokatly  
Physical Review A 93, 052515 (2016)

## Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra

J. Walkenhorst, U. De Giovannini, A. Castro, A. Rubio  
European Physical Journal B **89**, 128 (2016)

## Anisotropic electronic, mechanical and optical properties of monolayer WTe<sub>2</sub>

E. Torun, H. Sahin, S. Cahangirov, A. Rubio, F. M. Peeters  
Journal Of Applied Physics **119**, 074307 (2016)

In addition, the work that was performed under this grant was instrumental in assisting us, directly or indirectly, in obtaining the following nine prestigious Marie Skłodowska-Curie grants:

Marie Curie Intra-European Fellowships (IEF) (FP7-PEOPLE-2013-IEF, Project 622934) "Optical charge transfer processes in early stages of photosynthesis from first-principle computational techniques" (OptChaTra) Dr. Hannes Huebener (2014-2016). (Total: 166,336€)

Marie Curie Intra-European Fellowships (IEF) (FP7-PEOPLE-2013-IEF, Project 628876 "Photophysics of Fluorescent Proteins" (PhotoProtein). Dr. Seymour Cahangirov (2014-2016)- (Total: 173,370€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2014, Project 660231 "Electrical Spin Manipulation in Atoms and Molecules" (SpinMan). Dr. Andrea Droghetti (2016-2018). (Total: 158,122€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2014, Project SEP-210195067 "Quantum Effects in Multicolor Ultrafast Laser Processing: Broadening Boundaries of Classical Descriptions" (QuantumLaP). Dr. Derrien Thibault (2015-2017). (Total: 142,721€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 702406 "Correlated Electron-Nuclear Dynamics: A novel mixed quantum-semiclassical approach (CoEND)". Dr. Ali Abedi (2016-2018). (Total: 170,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 704218 "Strong Field Dynamics of Atoms and Molecules: History-dependent Functionals and Exact Kohn-Sham Potentials of the Time-dependent (multi-component) Density Functional Theory (AMO-dance)". Dr. Elham Khosravi (2016-2018). (Total: 170,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 706890 "Thermodynamics of Quantum Transport (QFluctTrans)". Dr. Cesar A. Rodriguez-Rosario (2016-2018). (Total: 170,121.60 €)



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Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 703195 "Spin-Orbit Coupling at Interfaces from Spintronics to new Superconducting effects (SOCISS)". Dr. Juan Borge de Prada (2016-2018). (Total: 158,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2016, Project 753874 "Excitonic quasiparticles in Titania (exciTania)". Dr. Adriel Dominguez (2017-2019). (Total: 158,121 €)

We greatly appreciate the support of the AOARD. Please contact grants manager Kate Chabarek ([kathryina.chabarek@ehu.eus](mailto:kathryina.chabarek@ehu.eus)) if you have any questions or concerns about the attached reports.

Many thanks.

Regards,



## Angel Rubio Distinguished Professor of Physics